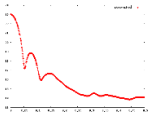
FoXS

Fast SAXS Profile Computation with Debye Formula



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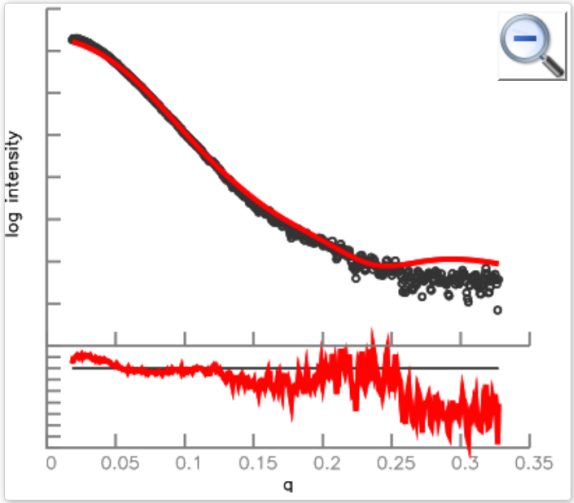
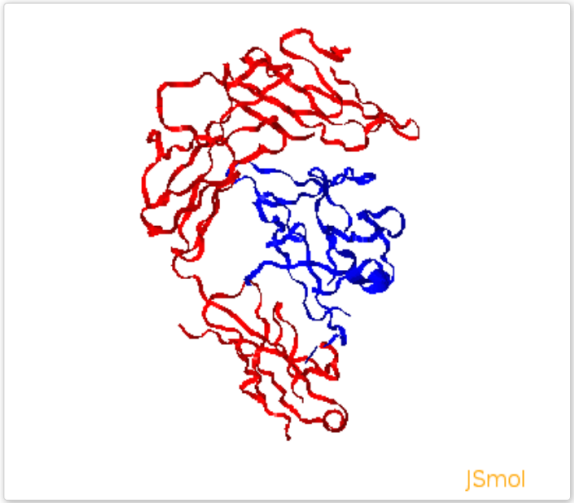
PDB files
4kc3AB.pdb

Profile file
complex.dat -

Can't see interactive display? Use old interface





PDB file	show/hide	χ	c_1	c_2	R_g	# atoms	fit file	png file
4kc3AB	☑	3.35	1.04	4.00	25.41	3288	4kc3AB_complex.dat	4kc3AB_complex.png

Figure S1: Fitting ST2-IL33 x-ray structure (PDB 4kc3) to the SAXS profile. The experimental and computed profiles are shown in black and red, respectively.

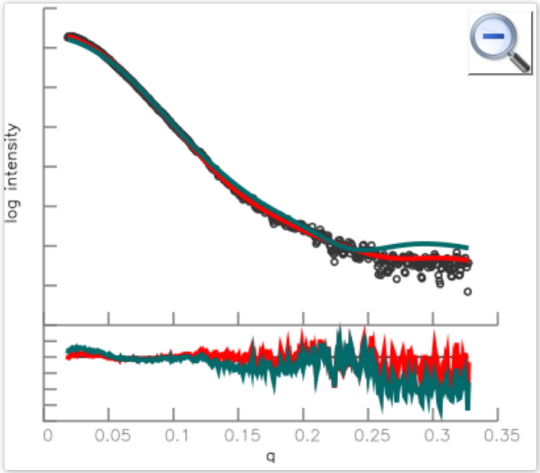
PDB files
complex_models.zip

Profile file
complex.dat -

Multi-state models by MultiFoXS Minimal Ensemble Search (MES) (about MES)

NEW! MultiFoXS Now with conformational sampling and multi-state modeling

Can't see interactive display? Use old interface

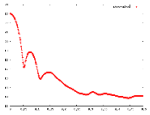


PDB file	show all/hide all	χ	c_1	c_2	R_g	# atoms	fit file	png file
st2_il33_5	☑	1.59	1.03	4.00	26.99	3730	st2_il33_5_complex.dat	st2_il33_5_complex.png
st2_il33_4	☐	1.62	1.03	4.00	26.93	3730	st2_il33_4_complex.dat	st2_il33_4_complex.png
st2_il33_2	☐	1.64	1.03	4.00	26.97	3730	st2_il33_2_complex.dat	st2_il33_2_complex.png
st2_il33_3	☐	1.65	1.03	4.00	26.80	3730	st2_il33_3_complex.dat	st2_il33_3_complex.png
st2_il33_6	☐	1.70	1.03	4.00	27.07	3730	st2_il33_6_complex.dat	st2_il33_6_complex.png
st2_il33_8	☐	1.74	1.03	4.00	26.84	3730	st2_il33_8_complex.dat	st2_il33_8_complex.png
st2_il33_9	☐	1.81	1.02	4.00	26.74	3730	st2_il33_9_complex.dat	st2_il33_9_complex.png
st2_il33_7	☐	1.87	1.03	4.00	26.40	3730	st2_il33_7_complex.dat	st2_il33_7_complex.png
st2_il33_1	☐	1.90	1.03	4.00	26.76	3730	st2_il33_1_complex.dat	st2_il33_1_complex.png
4kc3AB	☑	3.35	1.04	4.00	25.41	3288	4kc3AB_complex.dat	4kc3AB_complex.png

Figure S2: Fitting full length ST2-IL33 complex models based on the x-ray structure (PDB 4kc3) to the SAXS profile. The experimental profile is represented with black dots, the best scoring model (χ=1.59) and its profile are shown in red. For comparison, the x-ray structure and its profile are shown in green (χ=3.35).

FoXS

Fast SAXS Profile Computation with Debye Formula



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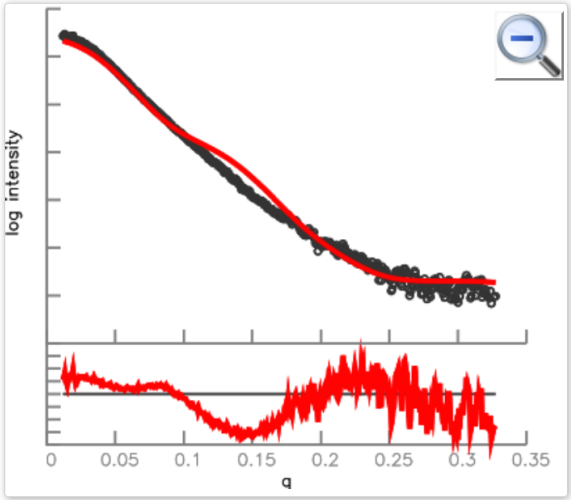
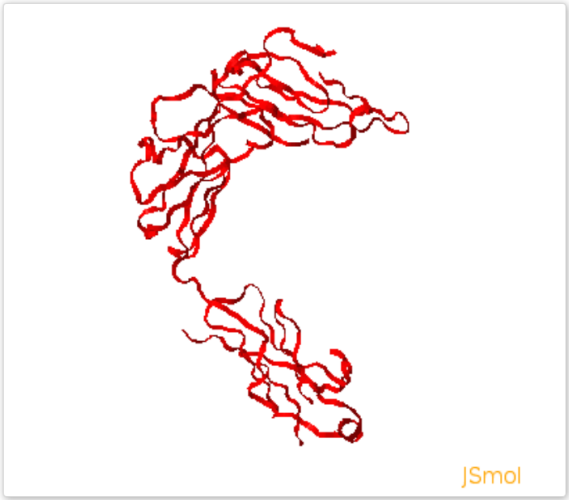
PDB files	Profile file	
4kc3B.pdb	st2.dat	-

Can't see interactive display? Use old interface





PDB file show/hide	χ	c_1	c_2	R_g	# atoms	fit file	png file
4kc3B ☑	7.72	1.05	4.00	28.34	2202	4kc3B_st2.dat	4kc3B_st2.png

Figure S3: Fitting ST2 x-ray structure (PDB 4kc3, chain B) to the SAXS profile. The experimental and computed profiles are shown in black and red, respectively.

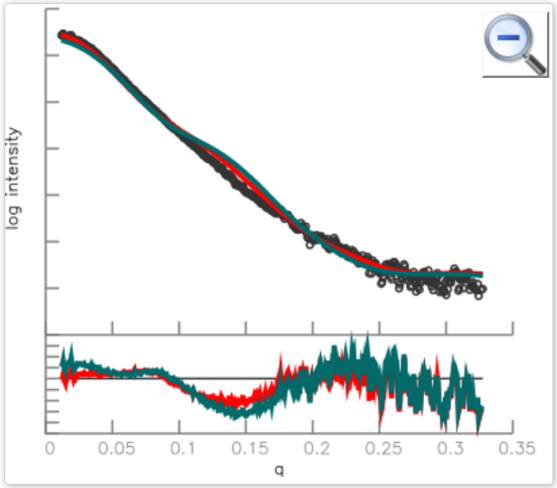
PDB files
st2_models.zip

Profile file
st2.dat -

Multi-state models by MultiFoXS Minimal Ensemble Search (MES) (about MES)

NEW! MultiFoXS Now with conformational sampling and multi-state modeling

Can't see interactive display? Use old interface



PDB file	show all/hide all	χ	c_1	c_2	R_g	# atoms	fit file	png file
st2_il33_2B	☑	5.54	1.05	4.00	30.44	2466	st2_il33_2B_st2.dat	st2_il33_2B_st2.png
st2_il33_1B	☐	5.85	1.05	4.00	30.24	2466	st2_il33_1B_st2.dat	st2_il33_1B_st2.png
st2_il33_5B	☐	5.91	1.05	4.00	30.44	2466	st2_il33_5B_st2.dat	st2_il33_5B_st2.png
st2_il33_6B	☐	6.19	1.05	4.00	30.62	2466	st2_il33_6B_st2.dat	st2_il33_6B_st2.png
st2_il33_4B	☐	6.21	1.05	4.00	30.44	2466	st2_il33_4B_st2.dat	st2_il33_4B_st2.png
st2_il33_9B	☐	6.55	1.05	4.00	30.20	2466	st2_il33_9B_st2.dat	st2_il33_9B_st2.png
st2_il33_8B	☐	7.11	1.05	4.00	30.34	2466	st2_il33_8B_st2.dat	st2_il33_8B_st2.png
st2_il33_3B	☐	7.13	1.05	4.00	30.25	2466	st2_il33_3B_st2.dat	st2_il33_3B_st2.png
st2_il33_7B	☐	7.27	1.05	4.00	29.78	2466	st2_il33_7B_st2.dat	st2_il33_7B_st2.png
4kc3B	☑	7.72	1.05	4.00	28.34	2202	4kc3B_st2.dat	4kc3B_st2.png

Figure S4: Fitting full length ST2 models based on the x-ray structure (PDB 4kc3) to the SAXS profile. The experimental profile is represented with black dots, the best scoring model (χ=5.54) and its profile are shown in red. For comparison, the x-ray structure and its profile are shown in green (χ=7.72).

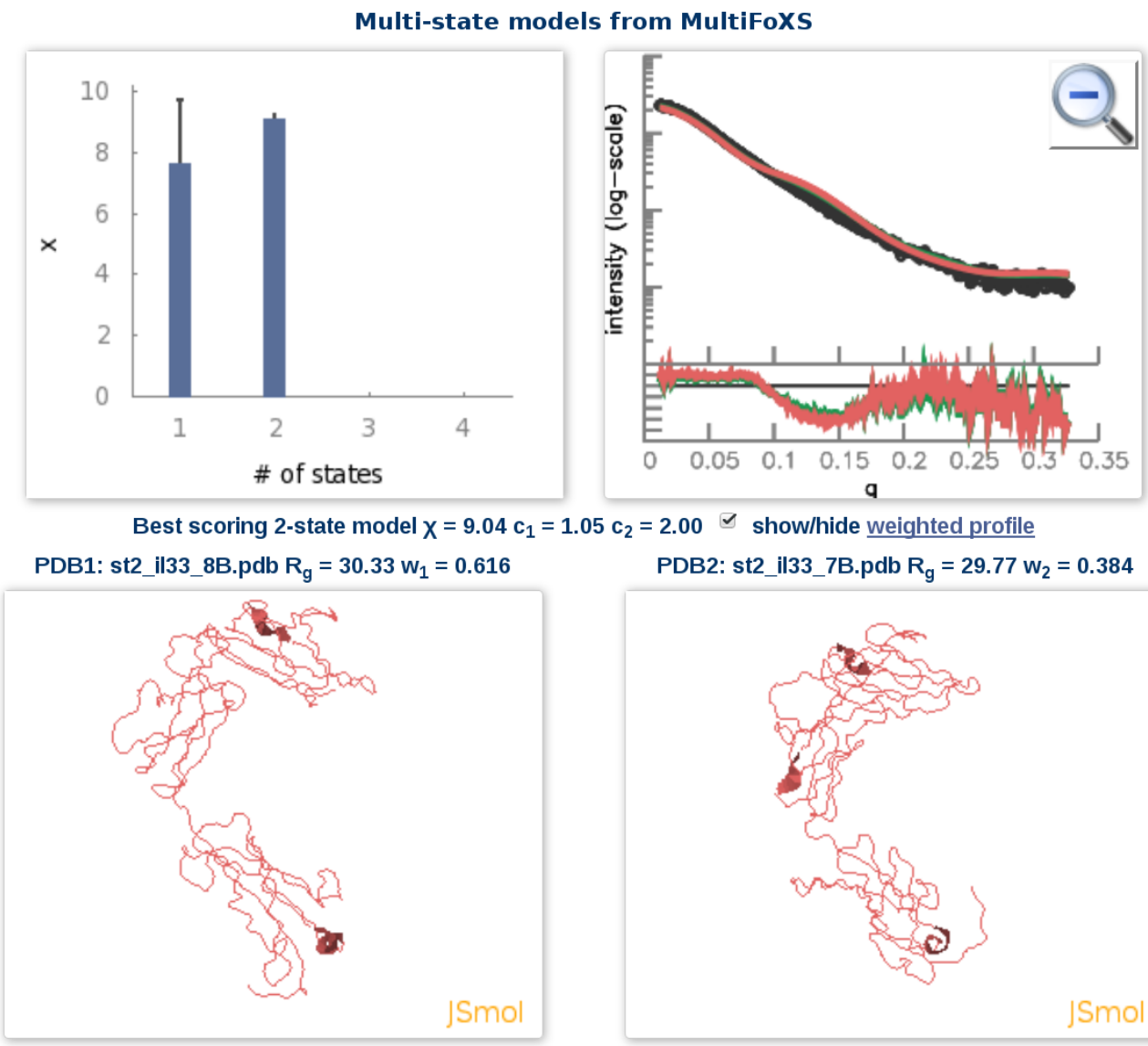


Figure S5: Multi-state models page on the FoXS server for ST2 models from previous figure. The bar plot and the fit plot are shown on top. The two state model is shown below. In this case multi-state modeling does not improve the fit to data because MODELLER models are very similar to each other.

A

FoXS Dock

Macromolecular Docking with SAXS Profile

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Receptor	Ligand	SAXS Profile	Complex Type
st2.pdb	2kll.pdb	complex.dat	Default

Model No	Z-Score	SAXS χ score	Energy score	Transformation	PDB file of the complex	
1	-4.787	1.390	-2018.849	0.84 0.59 -1.92 42.32 -40.93 17.45	result1.pdb	view
2	-4.671	1.439	-1951.717	0.96 0.34 -1.98 44.30 -40.07 19.12	result2.pdb	view
3	-4.618	1.888	-2028.433	-1.91 1.15 1.21 55.51 -35.51 -4.23	result3.pdb	view
4	-4.541	2.387	-2100.542	1.72 0.37 2.93 55.05 -39.65 7.12	result4.pdb	view
5	-4.379	1.666	-1808.728	1.03 0.37 -2.24 42.43 -42.70 18.02	result5.pdb	view
6	-4.376	1.304	-1716.199	1.15 0.43 -1.97 39.36 -41.71 16.97	result6.pdb	view
7	-4.265	1.678	-1734.010	0.53 0.47 -1.97 48.11 -42.25 17.23	result7.pdb	view
8	-4.254	2.483	-1928.365	-1.67 0.94 0.93 55.05 -37.69 -8.52	result8.pdb	view
9	-4.248	2.434	-1912.050	0.71 -1.40 2.77 51.67 -37.17 8.75	result9.pdb	view
10	-4.169	1.286	-1569.631	0.83 0.08 -2.10 40.12 -38.74 18.33	result10.pdb	view
11	-4.144	1.322	-1561.259	0.88 0.37 -1.89 40.53 -43.64 19.54	result11.pdb	view
12	-4.054	1.191	-1467.095	0.66 0.16 -1.76 42.06 -40.05 18.14	result12.pdb	view
13	-4.013	2.887	-1864.363	-1.47 0.72 0.44 56.35 -31.25 -6.28	result13.pdb	view
14	-3.978	1.760	-1557.778	0.82 0.61 -2.18 44.58 -40.84 16.09	result14.pdb	view
15	-3.974	1.893	-1589.181	1.85 0.04 -1.98 42.33 -41.89 21.59	result15.pdb	view
16	-3.922	2.119	-1609.988	-0.36 -0.63 0.85 36.29 -42.38 20.02	result16.pdb	view
17	-3.911	2.027	-1579.292	1.68 0.13 -2.02 47.14 -40.45 21.00	result17.pdb	view
18	-3.880	1.396	-1399.472	-0.94 0.84 -1.28 56.01 -39.26 4.83	result18.pdb	view
19	-3.827	1.577	-1408.993	2.00 0.07 -1.79 39.23 -42.29 21.40	result19.pdb	view
20	-3.814	2.018	-1510.772	-1.38 1.02 0.44 56.79 -29.62 -2.09	result20.pdb	view

»» show next 20

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B

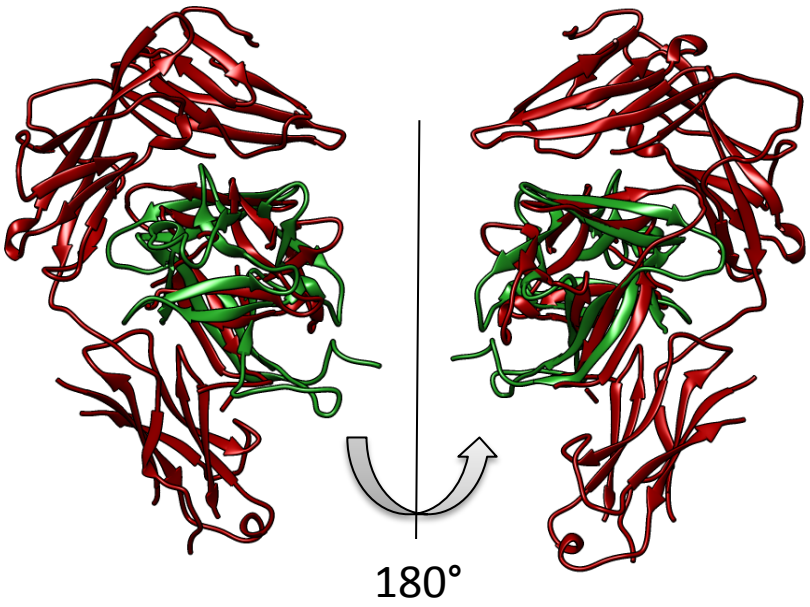
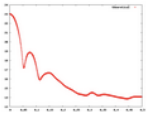


Figure S6: A) FoXSDock output page for docking ST2 to IL33. Each docking solution is shown with its final Z-score, χ score, and energy score. B) The top scoring solution (green) superimposed on the crystal structure (red) The superposition was performed using the ST2 chains.

FoXS

Fast SAXS Profile Computation with Debye Formula



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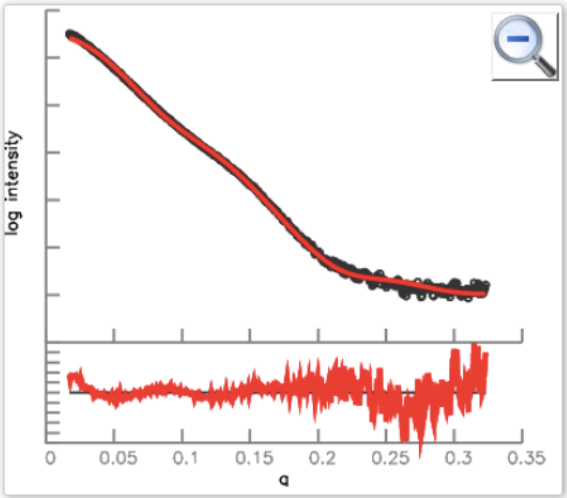
PDB files	Profile file	
1YJ5.pdb	pnk0.dat	-

Can't see interactive display? Use old interface



PDB file show/hide	χ	c_1	c_2	R_g	# atoms	fit file	png file
1YJ5 ☑	2.22	1.03	-0.85	29.71	3751	1YJ5_pnk0.dat	1YJ5_pnk0.png

Figure S7: Fitting mPNK x-ray structure (PDB 1yj5, chains B and C) to the SAXS profile. The experimental and computed profiles are shown in black and red, respectively.

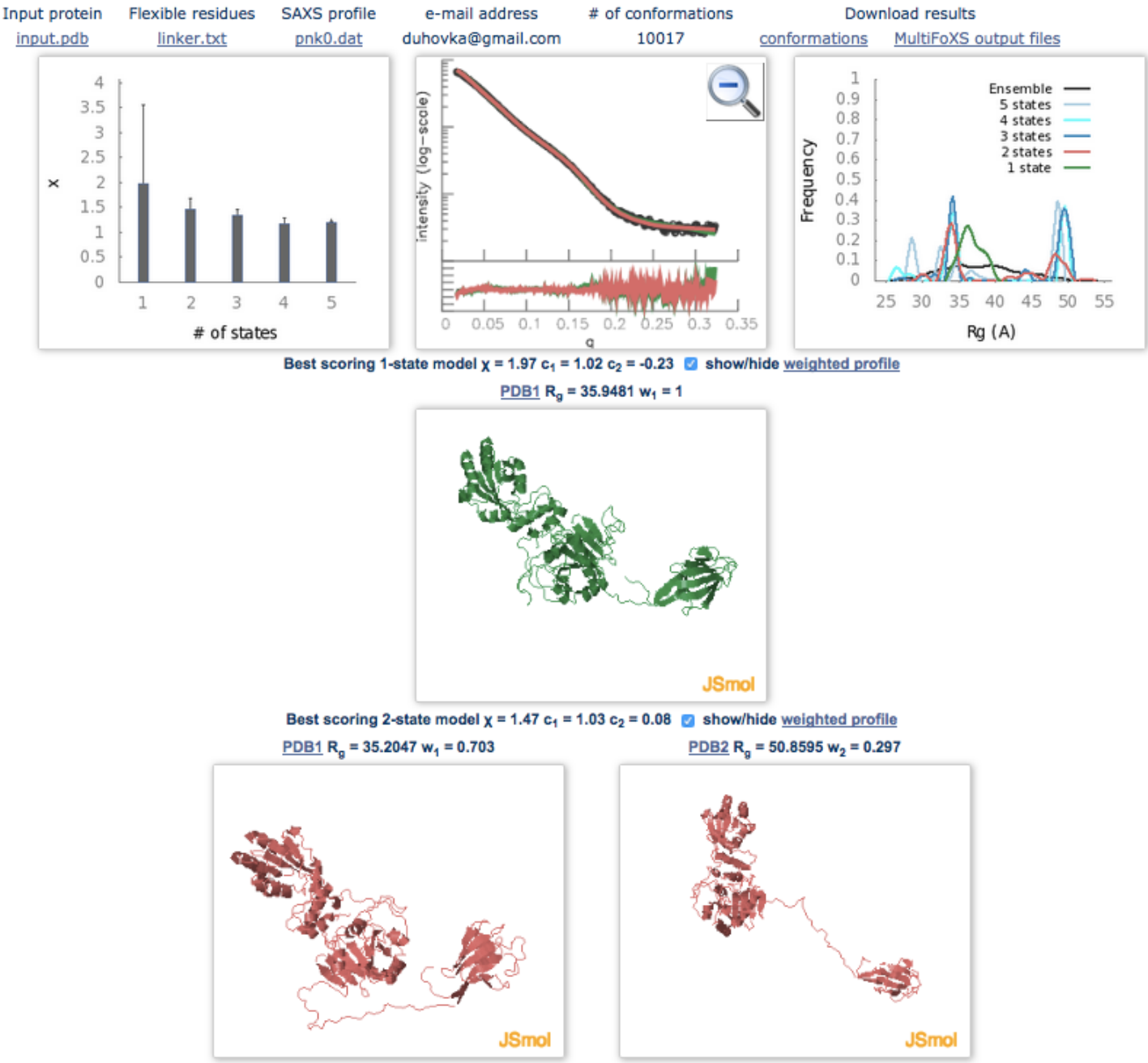


Figure S8. MultiFoXS output page for mPNK. The bar, fit, and *Rg* distribution plots are at the top. The top scoring one- and two-state models are shown in green and red, respectively.

A

FoXS Dock

Macromolecular Docking with SAXS Profile

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Receptor	Ligand	SAXS Profile	Complex Type
prot.pdb	dna.pdb	pkh1.dat	Default

Model No	Z-Score	SAXS χ score	Energy score	Transformation	PDB file of the complex	
1	-1.436	2.533	0.000	0.64 -0.12 -0.16 -12.24 51.91 -12.32	result1.pdb	view
2	-1.416	2.613	0.000	-0.36 -0.18 -0.25 -26.32 -0.21 31.76	result2.pdb	view
3	-1.383	2.745	0.000	0.22 0.16 0.07 12.35 10.58 -18.86	result3.pdb	view
4	-1.369	2.802	0.000	0.03 -0.11 0.07 -2.84 -3.19 2.59	result4.pdb	view
5	-1.336	2.937	0.000	-0.28 -0.00 0.08 2.53 -15.97 17.72	result5.pdb	view
6	-1.334	2.946	0.000	0.12 -0.15 -0.09 -17.82 10.00 -2.03	result6.pdb	view
7	-1.318	3.010	0.000	0.40 -0.15 -0.11 -17.56 31.83 -11.36	result7.pdb	view
8	-1.309	3.045	0.000	0.10 -0.35 0.09 -15.96 -0.56 12.55	result8.pdb	view
9	-1.300	3.084	0.000	0.13 -0.43 -0.05 -25.20 14.22 22.00	result9.pdb	view
10	-1.289	3.126	0.000	-2.39 -0.90 -1.92 35.89 23.63 134.89	result10.pdb	view
11	-1.287	3.133	0.000	-0.18 -0.47 -0.13 -27.92 0.57 35.72	result11.pdb	view
12	-1.281	3.161	0.000	-0.10 -0.04 0.09 -1.22 -9.09 6.29	result12.pdb	view
13	-1.279	3.168	0.000	0.30 -0.53 -0.26 -41.26 37.40 14.50	result13.pdb	view
14	-1.279	3.169	0.000	0.30 -0.08 0.13 -4.84 8.99 -18.24	result14.pdb	view
15	-1.262	3.238	0.000	-0.27 0.20 0.43 36.21 -27.59 2.96	result15.pdb	view
16	-1.231	3.360	0.000	0.03 -0.02 0.15 4.10 -3.74 1.68	result16.pdb	view
17	-1.231	3.362	0.000	-0.22 -0.08 0.06 0.17 -8.91 18.41	result17.pdb	view
18	-1.224	3.390	0.000	-1.28 -0.94 -1.16 -20.44 24.73 112.91	result18.pdb	view
19	-1.210	3.445	0.000	-0.55 -0.02 -0.04 -7.34 -16.03 36.69	result19.pdb	view
20	-1.192	3.519	0.000	-1.64 0.00 2.76 97.21 72.31 106.48	result20.pdb	view

»» show next 20

Download output file.

B

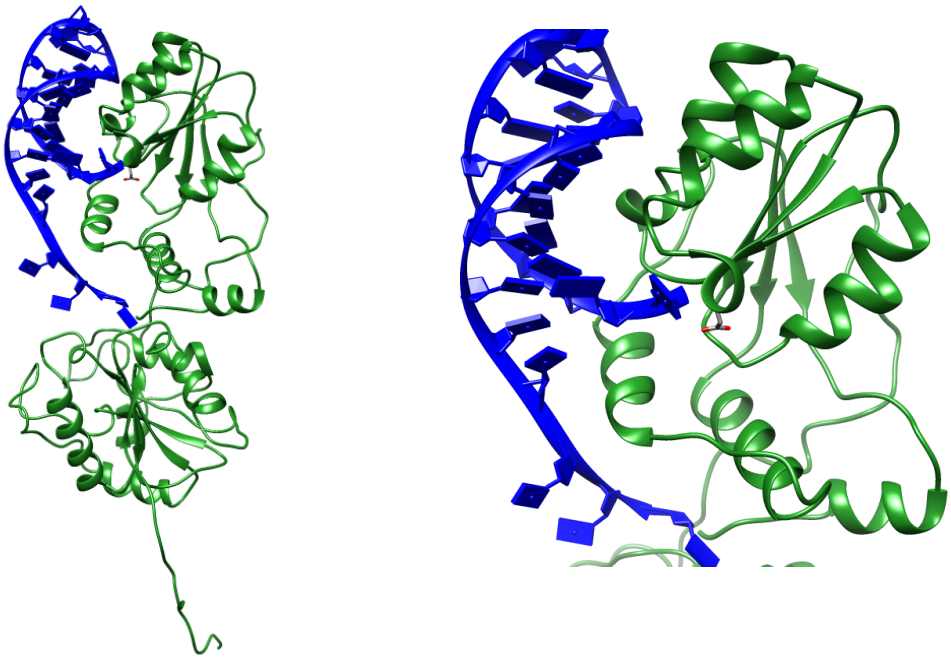

Figure S9: A) FoXSDock output page for docking mPNK catalytic domains to DNA. Each docking solution is shown with its final Z-score and χ score,. B) The top scoring model is consistent with known biochemical information, placing the ASP396 in close proximity to the 5'-hydroxyl group of the DNA substrate.